LECTURE 1

INTRODUCTION

Formulating a "Mathematical" Model versus a Physical Model

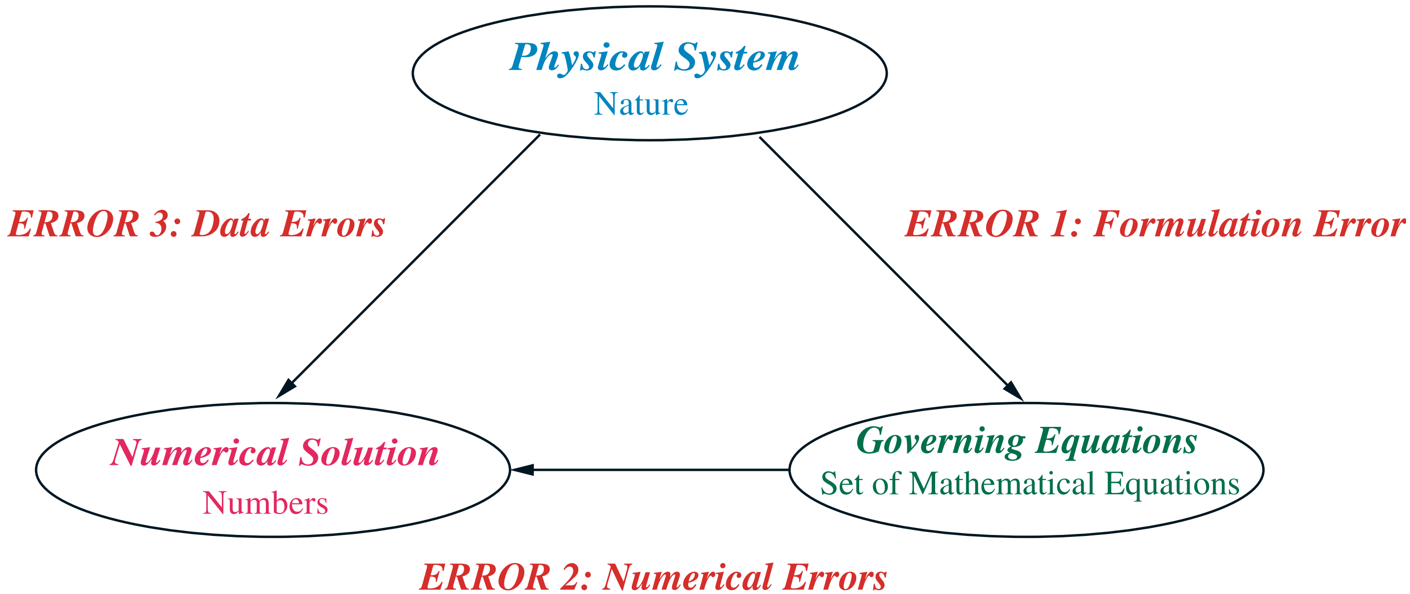
- Formulate the fundamental conservation laws to mathematically describe what is physically occurring. Also define the necessary constitutive relationships (relate variables based on observations) and boundary conditions (b.c.'s) and/or compatibility constraints.

- Use the laws of physics applied to an object/domain to develop the governing equations.
  - Algebraic equations
  - Integral equations → valid for the domain as a whole
  - p.d.e.'s → valid at every point within the domain
    - e.g. Newton's 2nd law applied to a point in a hypothetical continuum → Navier-Stokes equations

- Solve the resulting equations using
  - Analytical solutions
  - Numerical or discrete solutions

- Verify how well you have solved the problem by comparing to measurements

A MATHEMATICAL MODEL



- ***Engineering modelers should distinguish Formulation Errors, Numerical Discretization Errors and Data Errors***

Sources of Error in a Mathematical Solution

- Error 1: Missing or incorrect physics
  - Model doesn’t include an important process (e.g. forces due to surface tension)
  - Constitutive relationships are not a good approximation (e.g. friction law for pipes and channels not as applicable to the open ocean).
- Error 2: Numerical Solutions entail errors related to
  - Algorithm
  - Discretization
  - Boundary condition specification and domain selection
  - Computer type
- Error 3: Observational errors occur in
  - Measurements → e.g. instruments of limited accuracy
  - Data analysis techniques → e.g. techniques may not be appropriate or based on poor or invalid assumptions and approximations
  - Interpretation → e.g. are the right things being compared?

<u>Solutions to Governing Equations</u>

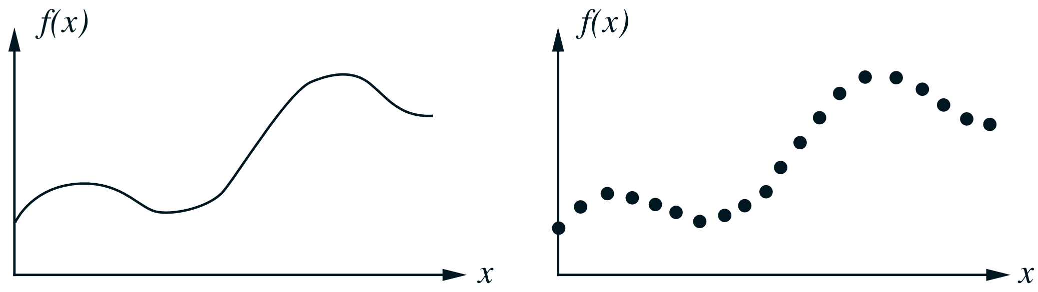
- It may be *very* difficult to solve a set of governing equations analytically (i.e. in closed form) for problems in engineering and geophysics.
- Governing equations may include
  - Nonlinearities
  - Complex geometries
  - Varying b.c.'s
  - Varying material properties
  - Large numbers of coupled equations
- These problems can not be solved analytically unless tremendous simplifications are made in the above aspects
- Simplification of governing equations
  - Lose physics inherent to the problem
  - Possibly a poor answer
- ***In general we must use numerical methods to solve the governing equations for real world problems***

Numerical Methods

- Used in hand calculations (many numerical methods have been around for hundreds of years)
- Used with computers (facilitate the type of operations required in numerical methods: Early 1940 $\rightarrow$ 1970: more developed 1970 $\rightarrow$ present)

How Numerical Methods Work

- Computers can only perform operations on numbers at discrete points in space/time
- ***Continuum representation of a function must be changed to a discrete representation***



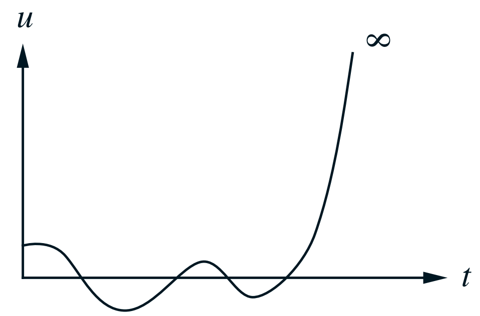
- Computers/compilers do not perform differential, integral or algebraic operations
- ***Differential, integral and algebraic operations must be transformed to arithmetic operations using discrete points***
- Numerical methods involve the representation and manipulation of governing equations in discrete arithmetic form
- There are many numerical methods for many tasks
    - To solve linear simultaneous algebraic equations
    - To solve nonlinear algebraic equations
    - To interpolate functions
    - To solve o.d.e.'s
        - i.v.p.'s
        - b.v.p.'s
    - To solve p.d.e.'s
    - To integrate functions
- Many of these techniques may have to be used to solve a single problem

Why Study Numerical Methods

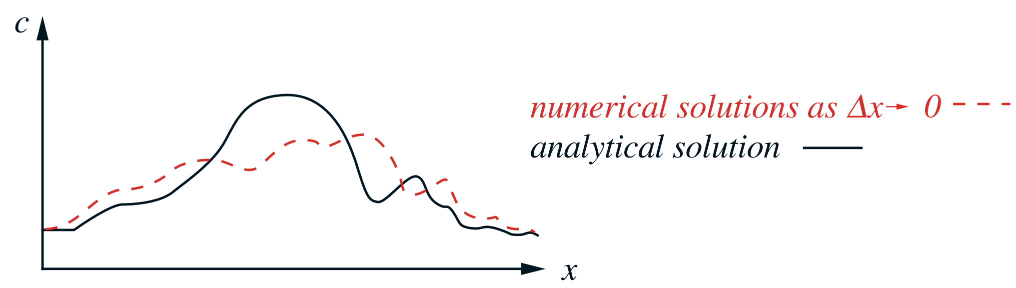
- No numerical method is completely trouble free in all situations!
  - How should I choose/use an algorithm to get trouble free and accurate answers?
- No numerical method is error free!
  - What level of error/accuracy do I have the *way* I'm solving the problem? → Identify error 2! (e.g. movement of a building)
- No numerical method is optimal for all types/forms of an equation!
  - Efficiency varies by orders of magnitude!!!
    - One algorithm for a specific problem → seconds to solve on a computer
    - Another algorithm for the same problem → decades to solve on the same computer
- ***In order to solve a physical problem numerically, you must understand the behavior of the numerical methods used as well as the physics of the problem***

Typical Difficulties Encountered with Numerical Methods

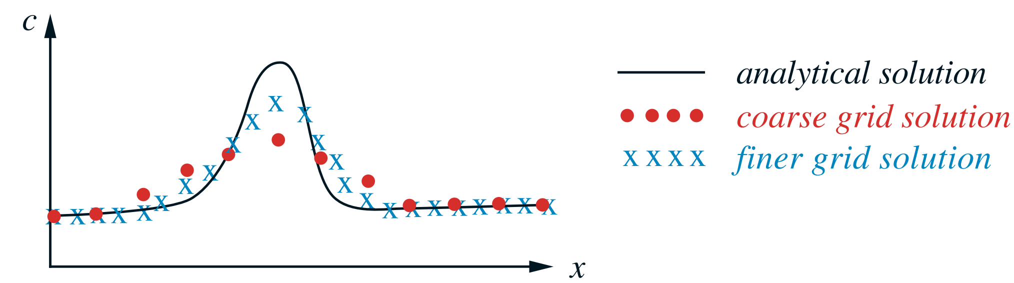
- The solution may become unstable



- The solution may be inconsistent
  - Even as the discretization size is made very small, the solution may never approach the hypothetical analytical solution to the problem!



- The solution may be highly inaccurate for a given discretization
  - This may result in significant under/over predictions of the solution



- ***An Engineer/Scientist as a developer and user must understand how a numerical method performs for his/her given problem.***

- An Engineer/Scientist must understand how various numerical algorithms are:
  - Derived
  - How the physics effects the numerics (e.g. nonlinearities) and how the numerics effects the physics (e.g. artificial damping)
  - Accuracy/stability properties (must use analysis techniques/numerical experiments)
  - Cost of a method for given level of accuracy (not per d.o.f.) → this varies substantially from method to method → computer memory, speed and architecture come into play as well

Example - Geophysical flows due to Tides and Winds in the Coastal Ocean

- Phenomena: Currents in the ocean and sea surface elevation are driven by wind, atmospheric pressure, variations in density (due to temperature/salinity variations) and by gravitational pull from the moon and sun (tides) and by Earth's gravity and wobble
- Interest:
  - Transport of pollutants (sewage, industrial toxics, heat waste, oil spills)
  - Transport of sediments (dredging, coastal erosion)
  - Sea surface elevation/currents (navigation, coastal flooding)
  - Both operational and design models exist
- Governing Equations

$$\frac{\partial \zeta}{\partial t} + \frac{\partial uH}{\partial x} + \frac{\partial vH}{\partial y} + \frac{\partial wH}{\partial \sigma} = 0$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial \sigma} - fv = -\frac{\partial}{\partial x}\left[\frac{p_s}{\rho_o} + g\zeta - \Gamma\right] + \frac{(a-b)}{H}\frac{\partial}{\partial \sigma}\left(\frac{\tau_{zx}}{\rho_o}\right) - b_x + m_x$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial \sigma} + fu = -\frac{\partial}{\partial y}\left[\frac{p_s}{\rho_o} + g\zeta - \Gamma\right] + \frac{(a-b)}{H}\frac{\partial}{\partial \sigma}\left(\frac{\tau_{zy}}{\rho_o}\right) - b_y + m_y$$

$$\frac{\partial p}{\partial \sigma} = -\frac{\rho g H}{(a-b)}$$

$$m_{x_\sigma} = \frac{1}{\rho_o}\left[\frac{\partial \tau_{xx}}{\partial x_\sigma} + \frac{\partial \tau_{yx}}{\partial y_\sigma}\right] - \frac{(a-b)}{H\rho_o}\left\{\left[\frac{\partial \zeta}{\partial x_\sigma} + \frac{(\sigma-a)}{(a-b)}\frac{\partial H}{\partial x_\sigma}\right]\frac{\partial \tau_{xx}}{\partial \sigma} + \left[\frac{\partial \zeta}{\partial y_\sigma} + \frac{(\sigma-a)}{(a-b)}\frac{\partial H}{\partial y_\sigma}\right]\frac{\partial \tau_{yx}}{\partial \sigma}\right\}$$

$$m_{y_\sigma} = \frac{1}{\rho_o}\left[\frac{\partial \tau_{xy}}{\partial x_\sigma} + \frac{\partial \tau_{yy}}{\partial y_\sigma}\right] - \frac{(a-b)}{H\rho_o}\left\{\left[\frac{\partial \zeta}{\partial y_\sigma} + \frac{(\sigma-a)}{(a-b)}\frac{\partial H}{\partial y_\sigma}\right]\frac{\partial \tau_{yy}}{\partial \sigma} + \left[\frac{\partial \zeta}{\partial x_\sigma} + \frac{(\sigma-a)}{(a-b)}\frac{\partial H}{\partial x_\sigma}\right]\frac{\partial \tau_{xy}}{\partial \sigma}\right\}$$

$$b_{x_\sigma} = \frac{g(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial x_\sigma} + \frac{g}{\rho_o(a-b)}\left| H\int_\sigma^a \frac{\partial \rho}{\partial x_\sigma} d\sigma - \frac{\partial H}{\partial x_\sigma}\int_\sigma^a (\sigma-a)\frac{\partial \rho}{\partial \sigma} d\sigma \right|$$

$$b_{y_\sigma} = \frac{g(\rho-\rho_o)}{\rho_o}\frac{\partial \zeta}{\partial y_\sigma} + \frac{g}{\rho_o(a-b)}\left| H\int_\sigma^a \frac{\partial \rho}{\partial y_\sigma} d\sigma - \frac{\partial H}{\partial y_\sigma}\int_\sigma^a (\sigma-a)\frac{\partial \rho}{\partial \sigma} d\sigma \right|$$

$$\eta(\lambda, \phi, t) = \sum_{n,\, i} C_{jn} f_{jn}(t_o) L_j(\phi) \cos[2\pi(t-t_o)/T_{jn} + j\lambda + V_{jn}(t_o)]$$

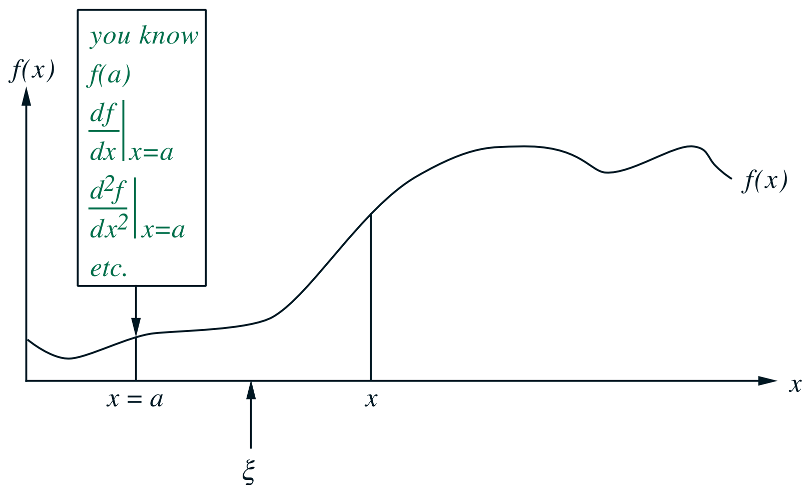
Taylor Series

- Many numerical **algorithms** are/can be derived from Taylor series
- Many **error estimates** are/can be based on Taylor series
- Taylor series is given as:

$$f(x) = f(a) + (x-a)\frac{df}{dx}\bigg|_{x=a} + \frac{(x-a)^2}{2!}\frac{d^2f}{dx^2}\bigg|_{x=a} + \frac{(x-a)^3}{3!}\frac{d^3f}{dx^3}\bigg|_{x=a} + \ldots + \frac{(x-a)^n}{n!}\frac{d^nf}{dx^n} + R$$

where

$$R = remainder = \frac{1}{(n+1)!}(x-a)^{n+1}\frac{d^{n+1}f}{dx^{n+1}}\bigg|_{x=\xi} \qquad a \le \xi \le x$$



- We can find the value of $f(x)$ at some $x \neq a$ if we remain sufficiently close to $x = a$ and if all the derivatives of f at $x = a$ exist.

- If we are too far away from $x = a$ $\rightarrow$ the Taylor series may no longer converge

    - A convergent series, converges to a solution as we take more terms (i.e. each subsequent term decreases in magnitude)

    - Some series will converge for all $(x - a)$ (radius of convergence), while for others there is a limit

    - If a series is convergent, then the value of $f(x)$ will be exact *if* we take an infinite number of terms (assuming no roundoff error on the computer)

- ***However we typically only consider the first few terms in deriving many numerical methods***

    - ***This defines the truncation error***

Example

- If we consider only the first two terms of the Taylor series, the neglected or truncated terms define the truncation error!

$$f(x) = f(a) + (x-a)\left.\frac{df}{dx}\right|_{x=a} + \frac{(x-a)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=a} + \frac{(x-a)^3}{3!}\left.\frac{d^3f}{dx^3}\right|_{x=a} + \ldots + \frac{(x-a)^n}{n!}\left.\frac{d^nf}{dx^n}\right|_{x=a}$$

- Various way of representing the truncation error

$$O(x-a)^2$$

$$\frac{(x-a)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=\xi} \qquad a \le \xi \le x$$

$$\frac{(x-a)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=a} + H.O.T.$$

- Note that the leading order typically dominates although the first few terms do sometimes compete.

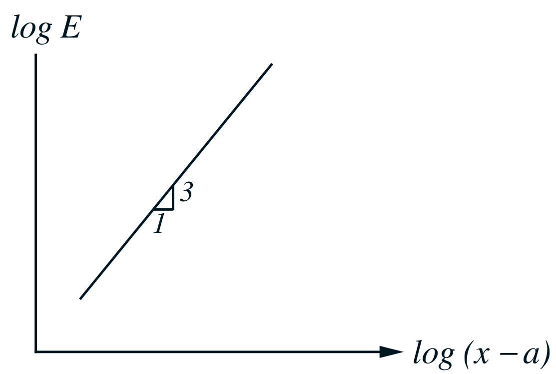
Example

- The accuracy of the series is determined by the order of the truncated error

$$f(x) = f(a) + (x-a)\left.\frac{df}{dx}\right|_{x=a} + \frac{(x-a)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=a} + O(x-a)^3$$

- $O(x-a)^3$ and all higher order terms are not considered

- $f(x)$ is accurate to $O(x-a)^3$ or third order accurate



Example

- Find the Taylor series expansion for $f(x) = \sin x$ near $x = 0$ allowing a 5th order error in the approximation:

$$f(x) = f(0) + (x-0)\left.\frac{df}{dx}\right|_{x=0} + \frac{(x-0)^2}{2!}\left.\frac{d^2f}{dx^2}\right|_{x=0} + \frac{(x-0)^3}{3!}\left.\frac{d^3f}{dx^3}\right|_{x=0}$$

$$+ \frac{(x-0)^4}{4!}\left.\frac{d^4f}{dx^4}\right|_{x=0} + O(x-0)^5 \quad \Rightarrow$$

$$f(x) = \sin(0) + x\cos(0) - \frac{x^2}{2!}\sin(0) - \frac{x^3}{3!}\cos(0) + \frac{x^4}{4!}\sin(0) + O(x)^5 \qquad \Rightarrow$$

$$\boldsymbol{f(x) = 0 + x - \frac{x^3}{3!} + O(x)^5}$$

SUMMARY OF LECTURE 1

- Numerical analysis always utilizes a discrete set of points to represent functions
- Numerical methods allows operations such as differentiation and integration to be performed using discrete points
- Developing/Using Mathematical-Numerical models requires a detailed understanding of the algorithms used as well as the physics of the problem!